Anomalously Soft Dynamics of Water in Carbon Nanotubes

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The structure and dynamics of water/ice confined to the 1-Dimensional nanotube interior are found to be drastically altered with respect to bulk water. Neutron diffraction, inelastic and quasielastic neutron scattering measurements in parallel with MD simulations (performed using the TTM2-F polarizable flexible water model with smeared charges and dipoles) have clearly shown the entry of water into open-ended SWNT and identified an ice-wall plus central water-chain structure. The observed extremely soft dynamics of nanotube-water/ice arises mainly from a qualitatively large reduction in the hydrogen-bond connectivity of the water-chain. An average coordination number of 1.86 was found due to continually breaking/forming of the hydrogen bonds between a water molecule with its nearest neighbors even at 50 K. Anomalously enhanced thermal motions in the water-chain, interpreted by a low-barrier, flattened, highly anharmonic potential well, explains the large mean-square displacement of hydrogen and fluid-like behavior of nanotube-water at temperatures far below the nominal freezing point.